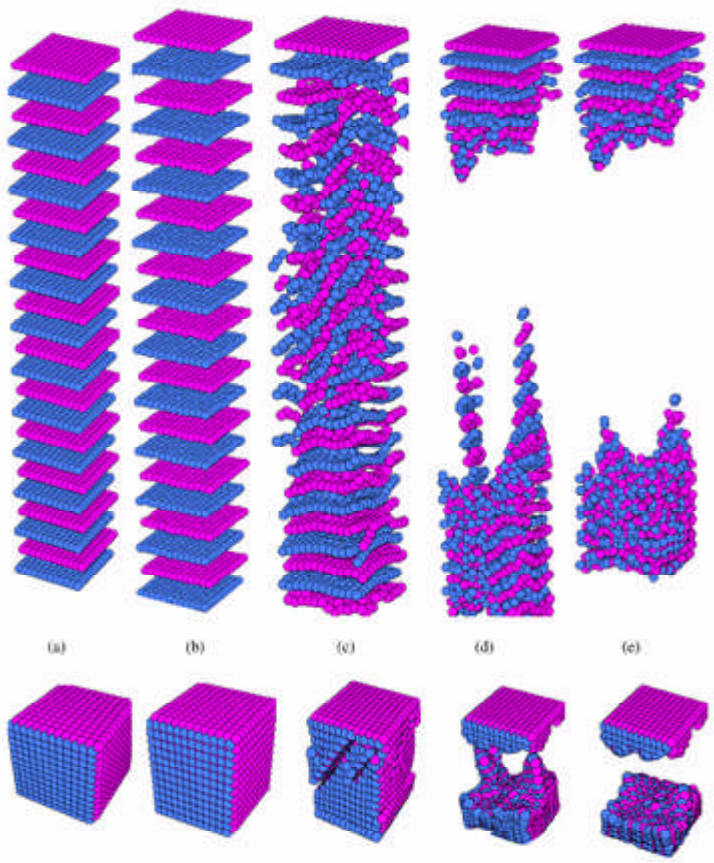
Monte Carlo Simulation of Alloy Design Techniques: Fracture and Welding Studied Using the BFS Method for Alloys

Large-scale simulations of dynamic processes at the atomic level have developed into one of the main areas of work in computational materials science. Until recently, severe computational restrictions, as well as the lack of accurate methods for calculating the energetics, resulted in slower growth in the area than that required by current alloy design programs.

The Computational Materials Group at the NASA Lewis Research Center is devoted to the development of powerful, accurate, economical tools to aid in alloy design. These include the BFS (Bozzolo, Ferrante, and Smith) method for alloys (ref. 1) and the development of dedicated software for large-scale simulations based on Monte Carlo-Metropolis numerical techniques, as well as state-of-the-art visualization methods. Our previous effort linking theoretical and computational modeling resulted in the successful prediction of the microstructure of a five-element intermetallic alloy, in excellent agreement with experimental results (refs. 2 and 3). This effort also produced a complete description of the role of alloying additions in intermetallic binary, ternary, and higher order alloys (ref. 4).

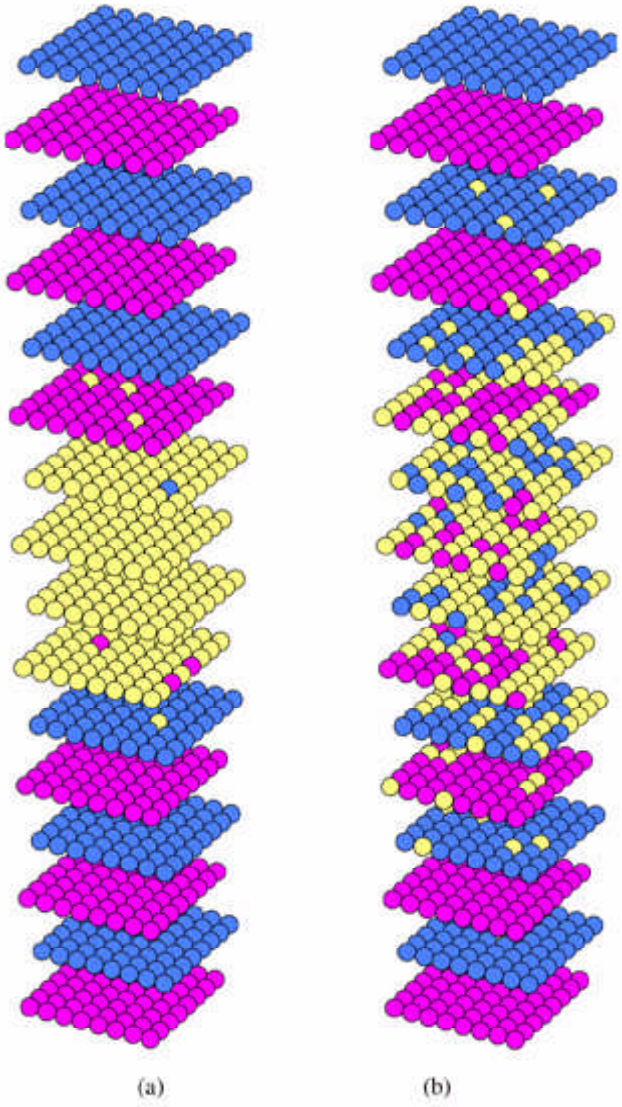


Onset of fracture for nickel aluminide (NiAl) for various states of the computational cell. Ni and Al atoms are denoted with red and blue spheres, respectively. (a) Beginning of the simulation. (b) After uniaxial strain, just before the onset of fracture. (c) Just after the onset of fracture. (d) During relaxation of the newly formed fracture surfaces. (e) After fracture relaxation is essentially complete.

A natural continuation of this work includes dynamic processes. Preliminary results from Monte Carlo-Metropolis minimization techniques used in conjunction with the BFS method for calculating the energetics, show a promising and viable way to gain insight into the microscopic evolution of intermetallic fracture, as shown in the preceding illustration. In this example, a nickel-aluminide- (NiAl) ordered alloy in the B2 phase is uniformly stretched until the computational cell develops cracks, which ultimately lead to the sample's fracture. Beyond this point, the surfaces thus created reconstruct, showing a strong preference for mixed-composition termination, as is to be expected. This Monte Carlo approach allows for individual atomic relaxations (which were exaggerated in the preceding illustration for visualization purposes).

The final illustration shows a temperature-dependent process where the computational cell is divided in two halves with an intermediate copper (Cu) layer, in what amounts to the first simulation of the brazing process. In this example, the temperature is raised steadily in small increments that allow the sample to stabilize at each step. The Monte Carlo-Metropolis approach used in this example allows only for atomic exchanges between

nearest neighbors, thus showing the increasing interdiffusion of Cu in the NiAl matrix as the temperature increases beyond the melting temperature of Cu.



NiAl + Cu computational cell. Ni, Al, and Cu atoms are denoted with red, blue, and yellow spheres, respectively. (a) Original cell, with four atomic layers of Cu between two identical NiAl cells. (b) After stabilization at 1400 °F.

Although Monte Carlo numerical techniques allow for a detailed visualization of the simulated process, the main advantage of this type of analysis is that it helps researchers to understand the underlying features that drive these processes. Because of the simplicity of the BFS method for the energetics used in these calculations, a detailed atom-by-atom analysis can be performed at any point in the simulation, providing necessary insight into the details of the process.

A main objective of this research program is to make the calculations as simple as possible. By reducing computational effort without losing physical accuracy, we expect

that powerful simulation tools will be developed in the immediate future which will allow material scientists to easily visualize and analyze processes at a level not achievable experimentally.

References

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